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September 29, 1998

Office of Naval Research
Program Officer Larry R. Cooper ONR 312
Ballston Centre Tower One
800 North Quincy Street
Arlington, VA 22217-5660

Subject: NAVY Grant No. N00014-98-1-0575

Dear Mr. Cooper:

On behalf of Dr. Albert-Laszlo Barabasi, the principal investigator for the subject grant, I am submitting three (3) copies of his Interim Performance Report with SF298. This report covers the period 06/01/98 thru 09/31/98.

If additional information is needed at this time, please do not hesitate to contact me. Thank you.

Sincerely,

Mary Ann Clark

for Howard T. Hanson, Director
Post Award Administration

HTH:mac

Encl.

cc: Director, NRL
Administrative Grants Officer, ONR
DTIC Office

PERFORMANCE REPORT FOR THE NAVY GRANT N00014-98-0575

Principal Investigator: Albert-László Barabási

In this report I describe work carried out from the interception on the Grant on 6/01/98 to the present.

Results:

(i) Ordering of the Self-Assembled Quantum Dots (SAQD): Two dimensional QD lattices

One of the primary goals of the purposed research was to predict theoretically the optimal growth conditions required for the creation of a perfect two-dimensional lattice of SAQDs. A major step in this direction was achieved in collaboration with my student, C. Lee. We have recently demonstrated that the combination of an ordered defect array with suitably chosen growth conditions for island formation has the potential to produce islands with properties that are superior to the currently grown samples. For this we calculated the effect of an impurity mesh on the island sizes and positions using atomistic Monte Carlo simulations. The simulations indicate that for a given pattern there exists an optimal set of growth conditions at which the error rate (the nucleation of an island at a position different from that determined by impurities) is the smallest and the most uniform islands form. We discussed the impact of these result on the growth of platelets and SAQDs. A paper about these results has been recently accepted for publication in Applied Physics Letters [1].

(ii) Dynamics of ripening of self-assembled II-VI semiconductor quantum dots

Parallel to this work, we have finished a joint experimental-theoretical work in collaboration with Professor Furdyna and Professor Merz on the ripening of the self-assembled quantum dots. In this work we reported a systematic investigation of ripening of CdSe QDs on ZnSe. Specifically, we investigated the properties of the CdSe islands (such as their density and size) as a function of time after deposition has been stopped. We find that strain is responsible for the remarkable uniformity of the island sizes at the end of the deposition process. However, despite the known effect of strain in stabilizing the size of the QDs, we have shown that the dynamics of the morphological changes which occur in CdSe QDs after growth is well described by the Ostwald ripening process. Furthermore, the experimental results allow us to identify the nature of the equilibrium growth mode characterizing the QD formation process, putting the results in the context of the equilibrium theory developed by us.

The paper on these results has been recently accepted for publication in Physical Review Letters [2].

(b) Work in progress

(i) A rather important question is how stress affects the island formation process. A better understanding of this problem is needed in order to take the proposed research program at the next level, and move form submonolayer islands to three dimensional islands. This work started last month, when my postoc, H. Jeong, hired recently and supported by this grant, started developing a three dimensional code for Monte Carlo simulations including stress. I expect that the development of this code will take months, but when it becomes functional, it will be the first Monte Carlo code with stress, and will allow us to achieve unparalleled understanding of the three dimensional island formation process.

(ii) A major component of the proposed work was the investigation of stacked self-assembled quantum dots. Along these lines, my student, Istvan Daruka, is currently spending six months in Los Alamos National Laboratory investigating, using molecular dynamics (MD) simulations, the stress in stacked quantum dots. Los Alamos has the capability of running over a hundred million particle MD simulations, enough to investigate islands with realistic sizes. The first results of this project are expected soon.

(iii) Finally, a collaboration between my student and J. Tersoff (IBM Watson Research Center) and myself is focused on investigating the shape of the self-assembled quantum dots theoretically. The conclusions of this work will be reported in future reports once the work it is completed.

5. Publications published or submitted with the support of the present grant:

[1] C. Lee and A.-L. Barabási, Spatial ordering of self-organized islands grown on patterned surfaces, *Applied Physics Letters (in press).*

[2] S. Lee, I. Daruka, C. S. Kim, A.-L. Barabási, J. L. Merz, and J. K. Furdyna, Self-organized growth and ripening of II-VI semiconductor quantum dots, *Physical Review Letters*, *(in press).*

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13. ABSTRACT *(Maximum 200 words)*
The research performed so far has provided two significant results. First, we demonstrated that the combination of an ordered defect array with suitably chosen growth conditions for island formation has the potential to produce islands with properties that are superior to the currently grown samples. Our simulations indicate that for a given pattern there exists an optimal set of growth conditions at which the error rate (the nucleation of an island at a position different from that determined by impurities) is the smallest and the most uniform islands form. Second, a joint experimental-theoretical work has focused on the ripening of the self-assembled quantum dots. We find that strain is responsible for the remarkable uniformity of the island sizes at the end of the deoposition process. We also find that the dynamics of the morphological changes which occur in QDs after growth is well described by the Ostwald ripening process. Work in progress includes the development of a three dimensional Monte Carlo simulation with strain, the investigation of stacked quantum dots using molecular dynamics, and research investigating the shape of self-assembled quantum dots.

14. SUBJECT TERMS
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